PACCON

PURE AND APPLIED CHEMISTRY INTERNATIONAL CONFERENCE 2009

PROCEEDINGS

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PURE AND APPLIED CHEMISTRY INTERNATIONAL CONFERENCE




JANUARY 14-16, 2009
NARESUAN UNIVERSITY, PHITSANULOK, THAILAND
Sustainable Development in Chemistry Based on Indigeneous Knowledge

PROFESSOR Dr.HER ROYAL HIGHNESS PRINCESS CHULABHORN

KEYNOTE SPEAKER

PURE AND APPLIED CHEMISTRY INTERNATIONAL CONFERENCE 2009

SUSTAINABLE DEVELOPMENT IN CHEMISTRY BASED ON INDIGENOUS KNOWLEDGE

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PROGRAM SUMMARY

TUESDAY: January 13th, 2009

Time	Akatodsarod 9 Room
13.00-17.00	**Registration** **Setting and Putting up Poster Presentation Session A** **3rd Floor Sirindhorn Building**

WEDNESDAY: January 14th, 2009

Time	Akatodsarod 9 Room
7.30-9.00	**Registration** **Setting and Putting up Poster Presentation Session A** **3rd Floor Sirindhorn Building**
9.10	**Opening ceremony** Guests are requested to be seated in the Akatodsarod 9
10.00	**Arrival of Professor Dr. Her Royal Highness Princess Chulabhorn**
10.05-10.15	• Present the Conference Package to Professor Dr. HRH Princess Chulabhorn by President of Chemical Society of Thailand • Report by the President of Naresuan University, the chairman of the Organizing Committee
10.15-10.25	**Professor Dr. Her Royal Highness Princess Chulabhorn graciously presents the Plaques of appreciation to 5 Plenary Lecturers, 3 Sponsors of PACCON 2009 and 6 recipients of the Wiley – CST Young Chemist Awards**
10.25-10.40	**Royal Opening Address by Professor Dr. HRH Princess Chulabhorn**
10.40-10.50	Introduction of Professor Dr. Her Royal Highness Princess Chulabhorn by Dean of Faculty of Science, Naresuan University
10.50-11.30	**Special Keynote Lecture by Professor Dr. Her Royal Highness Princess Chulabhorn**
11.40	**Professor Dr. Her Royal Highness Princess Chulabhorn has photographs taken with two groups of organizing committee**
12.00-13.30	**LUNCH** **Faculty of Science, Naresuan University** **Setting and Putting up Poster Presentation Session A** **3rd Floor Sirindhorn Building**
13.30-14.00	VDO presentations of Naresuan University, Pibulsongkarm Rajabhat University, and Rajamangala University of Technology Lanna and Introduction to PACCON
14.00-14.30	**Plenary lecture I** Chairperson: Supawan Tantayanon ***Peter Schwarz*** (Alexander-von-Humboldt High School, Germany) "Microscale Gas Experiments with Disposable Materials"

	"Analytical Chemistry, Chemical Analysis, and the Integration of Research with Teaching and Learning"
9.30-10.30	**Plenary lecture IV** Chairperson: Duangjai Nacapricha *Kate Grudpan* (Chiang Mai University, Thailand) "Is that (simple) Enough as a Ground for Biomedical and Green (analytical) Chemistry Applicable to Rural Places?"

PROGRAM SUMMARY

10.30-10.45	**Coffee Break**

ORAL PRESENTATION
Jan 15th 2009

	Akatodsarod 1 Room	Akatodsarod 2 Room	Akatodsarod 3 Room	Akatodsarod 4 Room	Akatodsarod 5 Room	Naresuan 1 Room	Naresuan 2 Room	Naresuan 3 Room	Naresuan 4 Room
	S 16 **Renewable Energy**	S1 **Analytical Chemistry**	S3-S6 **Organic chemistry(S3) Medicinal Chemistry(S6)**	S8 **Biological and Biophysical Chemistry**	S12 **Environmental Chemistry and Chemical Engineering**	S7 **Material Science and Nanotechnology**	S7 **Material Science and Nanotechnology**	S10 **Polymer Chemistry**	S5 **Chemical Education**
10.45-11.15	**Invited Lecture** **S16-INV-1:** **Dusit Kruanggam**	**Invited Lecture** **S1-INV-1** **Proespichaya Kanatharana**	**Invited Lecture** **S3-INV-1** **Mongkol Sukwattanasinitt**	**Invited Lecture** **S8-INV-1** **Pallop Karnchanaphanurach**	**Invited Lecture** **S12-INV-1** **Puangrat Kajitvichyanukul**	**Invited Lecture** **S7-INV-1** **Teerakiat Kerdcharoen**	**Invited Lecture** **S7-INV-2** **Geoffrey Mitchell**	**Invited lecture** **S10-INV-1** **Pranee Phinyocheep**	S5-OR-1 S5-OR-2
11.15-12.30	S16-OR-1 S16-OR-2 S16-OR-3 S16-OR-4	S1-OR-1 S1-OR-2 S1-OR-3 S1-OR-4 S1-OR-5	S3-OR-1 S3-OR-2 S3-OR-3 S6-OR-1 S6-OR-2	S8-OR-1 S8-OR-2 S8-OR-3 S8-OR-4	S12-OR-1 S12-OR-2 S12-OR-3 S12-OR-4 S12-OR-5	S7-OR-1 S7-OR-2 S7-OR-3 S7-OR-4 S7-OR-5	S7-OR-6 S7-OR-7 S7-OR-8 S7-OR-9 S7-OR-10	S10-OR-1 S10-OR-2 S10-OR-3 S10-OR-4 S10-OR-5	S5-OR-3 S5-OR-4
12.30-14.00	**LUNCH** **Faculty of Science, Naresuan University** **Setting and Putting up Poster Presentation Session B** **3rd Floor Sirindhorn Building**								
	Akatodsarod 1 Room	**Akatodsarod 2 Room**	**Akatodsarod 3 Room**	**Akatodsarod 4 Room**	**Akatodsarod 5 Room**	**Naresuan 1 Room**	**Naresuan 2 Room**	**Naresuan 3 Room**	**Naresuan 4 Room**
	S 16 **Renewable Energy**	**S1** **Analytical Chemistry**	**S6-S14** **Medicinal Chemistry(S6) Industrial Chemistry and Innovation(S14)**	**S8-S9** **Biological and Biophysical Chemistry & Bioinformatics/ Cheminformatics**	**S12** **Environmental Chemistry and Chemical Engineering**	**S7** **Material Science and Nanotechnology**	**S7** **Material Science and Nanotechnology**	**S10** **Polymer Chemistry**	
14.00-14.30	S16-OR-5 S16-OR-6	**Invited Lecture** **S1-INV-2** **Waraporn Som-aum**	**Invited Lecture** **S14-INV-1** **Sanong Ekgasit**		**Invited Lecture** **S12-INV-2** **Suparoek Henpraserttae**			**Invited Lecture** **S10-INV-2** **Shinzo Kohjiya**	
14.30-15.45	S16-OR-7 S16-OR-8 S16-OR-9 S16-OR-10	S1-OR-6 S1-OR-7 S1-OR-8 S1-OR-9 S1-OR-10	S6-OR-3 S6-OR-4 S14-OR-1 S14-OR-2	S8-OR-5 S8-OR-6 S8-OR-7 S9-OR-1 S9-OR-2	S12-OR-6 S12-OR-7 S12-OR-8 S12-OR-9 S12-OR-10	S7-OR-11 S7-OR-12 S7-OR-13 S7-OR-14 S7-OR-15	S7-OR-16 S7-OR-17 S7-OR-18 S7-OR-19 S7-OR-20	S10-OR-6 S10-OR-7 S10-OR-8 S10-OR-9	
15.45-16.00	**Coffee break**								

12.00-12.15	S2-OR-4	**Leenawat Kanda,** Synthesis of High Surface Area Molybdenum Oxide Supported Silica Catalyst by Sol gel Method
12.15-12.30	S2-OR-5	**Suttipong Wannapaiboon**, Influences of Ultrasonic Wave Activation on Phase Formation and Characteristics of Barium Zirconate Powders Under Ammonothermal Conditions
12.30-12.45	S2-OR-6	**Peerathat Pinpithak**, Synthesis and Characterization of Metal Doped Mesoporous Titania for Dye-Sensitized Solar Cell Application
12.45-13.00	S2-OR-7	**Cahyorini Kusumawardani**, Surface Modification of TiO_2 Films with Nanosized CdS and Its Characterisation for Dye-Sensitised Solar Cells Application

Oral Presentation Schedule

Akatodsarod 4 Room		
Chairperson: Thawatchai Tantulani		
14.00-14.30	S2-INV-2	**Korakot Navakhun,** Deprotonation Reactions of the Non-Rigid Bis-(2,5-diamidopyrrole) Induced by Anions
14.30-14.45	S2-OR-8	**Wanwisa Janrungroatsakul**, Fabrication of Silver Selective Microelectrodes for Submicromolar Detections
14.45-15.00	S2-OR-9	**Matinee Jamkratoke**, Fluorescent Methods for Determination of Micromolar Concentrations of the Cyanide Ion in Aqueous Micellar Systems
15.00-15.15	S2-OR-10	**Nisachol Nerngchamnong**, Ditopic Anion Electrochemical Sensors Containing Calix[4]Arenes
15.15-15.30		**Coffee break**
15.30-15.45	S2-OR-11	**Natthawat Semakul**, Hydrothermal Preparation and Characterization of Refractory Pigment Based on Perovkite Cobalt Titanate
15.45-16.00	S2-OR-12	**Sayekti Wahyuningsih**, Enhancement of Visible Oxidation Photocatalytic by Adsorption of Pyridilazoresorcinol Complexes onto Mesopore TiO_2
16.00-16.15	S2-OR-13	**Klit Toonkat**, The Effect of Chemical Additives on the Performance of Activated Carbon Adsorbent Bed
16.15-16.30	S2-OR-14	**Krit Lertjiamratn,** Dehydration of Methanol to Dimethyl Ether on Mixed Phases Alumina
S 3: Organic Chemistry		
January 15th, 2009	**Akatodsarod 3 Room**	
Chairperson: Chanitsara Sriwattanawarunyoo		
10.45-11.15	S3-INV-1	**Mongkol Sukwattanasinitt**, Molecular Engineering of Photoactive Organic Materials
11.15-11.30	S3-OR-1	**Abbas Teimouri**, Synthesis of Mono and Bis-Morpholiniummethyl-urea as Corrosion Inhibitors for Steel in Acidic Media.
11.30-11.45	S3-OR-2	**Komsan Imphanban**, Synthesis of *N*-Formylnornuciferine and *N*-Formylannonaine by Palladium Catalysis.
11.45-12.00	S3-OR-3	**Siwarutt Boonyarattanakalin**, Convergent Synthesis of Phosphatidylinositol Hexamannoside Glycan of Mycobacterium tuberculosis.
S 4: Physical and Theoretical Chemistry		
January 16th, 2009	**Akatodsarod 3 Room**	
Chairperson: Siriporn Jungsuttiwong		
10.45-11.15	S4-INV-1	**Vudhichai Parasuk**, Stereoselectivity of Catalyzed Mannich Reaction: Comparision between Proline and Thioproline Catalyst
11.15-11.30	S4-OR-1	**Janchai Yana,** Molecular Dynamics Simulations of Ion Bombardment on Nafion Side Chain Cluster Model
11.30-11.45	S4-OR-2	**Panthip Tue-ngeun**, Molecular Dynamics of Single-Chain Antibody to HIV Epitope at C-Terminal of P17
11.45-12.00	S4-OR-3	**Uthumporn Arsawang,** Molecular Dynamics Simulations and Quantum Chemical Calculations of GEMZAR® in Functionalized Carbon Nanotube
12.00-12.15	S4-OR-4	**Purinchaya Sornmee,** Molecular Dynamics Simulations of Doxrubicin Encepsulated in Single-Walled Carbon Nanotube
12.15-12.30	S4-OR-5	**Oranit Phuakkong,** Structure and Reaction Mechanisms of Peptide Formation over Nanostructured Zeolite
12.30-12.45	S4-OR-6	**Tammarat Piansawan**, Theoretical Study of Mechanism and Kinetics for the Reaction of Chlorine Atoms with Toluenes
12.45-13.00	S4-OR-7	**Sittichoke Tabthong,** A Theoretical Study of the Ring-Opening Mechanism of Lactide Initiated by a Tetradentate Bis(pyrrole) Schiff Base Aluminium Complex
January 16th, 2009	**Akatodsarod 3 Room**	
Chairperson: Vudhichai Parasuk		
14.00-14.15	S4-OR-8	**Suranan Anantachaisilp**, Physicochemical Characterization of Gamma-Oryzanol Encapsulated in Solid Lipid Nanoparticles (SLN), Nanostructured Lipid Carriers (NLC), and Nanoemulsion (NE)
14.15-14.30	S4-OR-9	**Luckhana Lawtraku**, Quantitative Structure-Thermodynamics Property Relationship of Host-Guest Cyclodextrin Inclusion Complexes
14.30-14.45	S4-OR-10	**Fumio Tanaka**, Correlation between Photoinduced Electron Transfer Rate and Structural Factors in FMN Binding Protein
14.45-15.00	S4-OR-11	**Siriporn Jungsuttiwong**, Characterization of Acidic Positions and Acidity in Isomorphous Substituted ZSM-5: Embedded DFT/UFF and DFT Approaches
15.00-15.15	S4-OR-12	**A. Kazemi Babaheydari**, The Adsorption H2 on Vanadium (100) Surface
15.15-15.30	S4-OR-13	**M. T. baei**, DFT Study Threonine Amino Acid with Cadmium Cation and Formation of Complexes the $[Cd\text{-}(Thr)_{n=(1\text{-}3)}]^{2+}$
S 5 : Chemical Education		
January 15th, 2009	**Naresuan 4 Room**	
Chairperson: Prasak Thavornyutikarn		
10.45-11.00	S5-OR-1	**Suyanta Rr.,** Structured Clock Reaction Demonstration Implementation on Assessing Student's Understanding of Atomic Structure, Chemistry Bond, Thermochemistry, and Acid and Base Concepts
11.00-11.15	S5-OR-2	**Norita Mohamed**, Development of Microscale Chemistry in Malaysia
11.15-11.30	S5-OR-3	**Jose H. Bergantin, Jr**, Low-Cost Cear-Box Microscale Digital Polarimeter
11.30-11.45	S5-OR-4	**Joyce T. Tan,** Low Cost pH Sensor for Microscale Experiments

THE STUDY OF CROSSED ALDOL CONDENSATION AT THE SYNTHESIS OF ASYMMETRIC DIBENZALACETONE

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Abstract: The synthesis of asymmetric dibenzalacetone has been done by crossed aldol condensation. It can be made from 3,4-dimethoxybenzaldehyde, benzaldehyde and acetone as the starting materials. As a nucleophile, acetone, has α-hydrogens in two side. So, it can attack two kinds of aldehydes. The product will be characterized by ^{1}H-NMR, ^{13}C-NMR, HMQC and HMBC spectrometer. Therefore, it was identified as 1(E),4(E)-1-phenyl-5-(3',4'-dimethoxyphenyl)-penta-1,4-diene-3-one.

Introduction

Aldol Condensation is occured by a nucleophilic addition of the enolate ion to a carbonyl. Acetone also undergoes aldol condensation, but the equilibrium concentration of the product is generally small. Cross aldol condensation between *p*-annisaldehyde from fennel oil with acetophenone produce 2-hydroxy-4-methoxychalcone [1]. The influence of the base concentration and reaction time on the cross aldol condensation reaction also has been reported [2]. Alnustone or 4(E),6(E)-1,7-diphenyl-4,6-heptadiene-3-one is an asymmetric compound that isolated from Curcuma xanthorrhiza (*Zingiberaceae*). This compound was synthesized by Goksu, et al. using crossed aldol condensation between benzaldehyde and acetone, followed by reaction with cinnamaldehyde [3].

Handayani and Arty have synthesized 1.5-diphenyl-penta-1,4-diene-3-one and its derivatives known as symmetrical dibenzalacetone. It made by crossed aldol condensation between acetone : benzaldehyde by 1:2 mol ratio. It also tested as a radical hydroxyl scavengers [4]. Asymmetric crossed aldol condensation have been done with various catalyst [5,6,7]. Tutik D had synthesized of a symmetrical dibenzalacetone that have a similar structure with the cinnamic acid derivatives[8]. From its structure, it is estimated that benzalacetone and dibenzalacetone will absorb ultraviolet in the same range. Thus, asymmetric dibenzalacetone will act as a radical scavenger and also a sun screen. In this research asymmetric dibenzalacetone, compound **5** namely 1(E),4(E)-1-phenyl-5-(3',4'-dimethoxyphenyl)-penta-1,4-diene-3-one will be synthesized. This compound was made by crossed aldol condensation between acetone with two aldehydes which are the benzaldehyde and 3.4-dimethoxybenzaldehyde.

Materials and Methods

General . All materials were from Merck, among other acetone, benzaldehyde, 3.4-dimethoxybenzaldehyde, ethanol, chloroform, hexane, and ethyl acetate. TLC was carried out using 0.25-mm plate Silica gel Merck 60 F254, column chromatography were performed by Silica gel 60 (230-400 mesh). The ^{1}H-NMR, ^{13}C-NMR, HMQC and HMBC spectra were recorded on 500 MHz Jeol instrument. IR spectra were conducted using a Shimadzu 8300 FTIR spectrometer.

1(E),4(E)-1-phenyl-5-(3',4'-dimethoxyphenyl)-penta-1,4-diene-3-one (5). Into a solution of NaOH (0.025 mol, 1g) in aqueous ethanol (1:1) that was prepared at ambient temperature, benzaldehyde (0.01 mol, 1.06 g), acetone (0.01 mol, 0.58 g) and 3,4-dimethoxybenzaldehyde (0.01 mol, 1.66 g) were added drop wise alternately. After additional stirring for 60 minutes, water (20 ml) was added to the reaction mixture which was then filtered. The extract was washed with water (20 ml x 3) and separated by column chromatography (d 2.5 cm, h 50 cm), with silica gel 60 (230-400 mesh) as the stationary phase and ethylacetate-hexane by 1:9 as the eluent. Four fractions were obtained from the column chromatography. The target compound was identified using thin layer chromatography with chloroform-hexane 4: 6.

Results and Discussion

Improved Synthesis of 1(E),4(E)-1-phenyl-5-(3',4'-dimethoxyphenyl)-penta-1,4-diene-3-one (5). The preparation of compound **5** was initiated by the mixing of **1, 2** and **4** to give **5** ((Figure 1). The product of crossed aldol condensation between benzaldehyde, 3,4-dimethoxybenzaldehyde and acetone is a mixture of 4 compounds. There was separated by Column Chromatography (EtOAc-hexane, 1:9) to provide the asymmetric dibenzalacetone **5** (15.53%) as pale yellow oil.

The multiple bond correlation of HMBC supported the structure (Table 1, Figure 2). In the ^{1}H-NMR spectrum (500 MHz, $CDCl_3$), three protons singlet and three protons double dublet were observed. The singlet at δ = 7.37 was assignable to H2', 3.8 to H3' and 3.9 to H4'. The double dublet at δ = 7.2; 7.63; and 6.9 was

assignable to H3", H4" and H5" respectively. Two equivalence methoxy signals at δ 3.8 and 3.9 were assigned to C3' and C4'. Support spectra data provided by the IR (KBr), which indicates the existence of C=O (1645cm^{-1}), aromatic C=C (1514-1417 cm^{-1}) and CO ether (1255-1139 cm^{-1}). Therefore, the structure of **5** was 1(E),4(E)-1-phenyl-5-(3',4'-dimethoxyphenyl)-penta-1,4-diene-3-one.

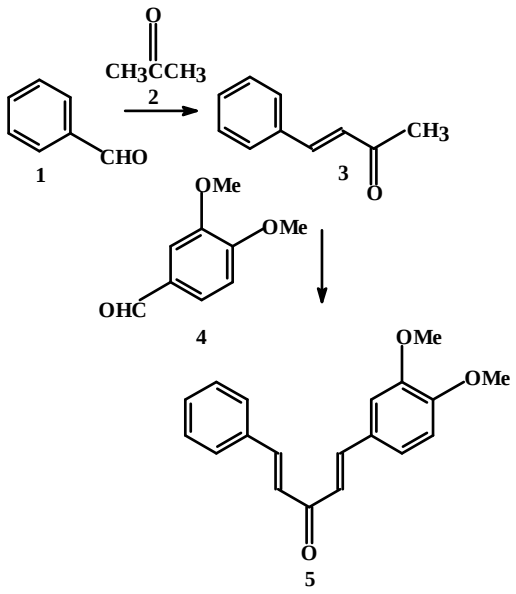

Figure 1. Synthesis of 1(E),4(E)-1-phenyl-5-(3',4'-dimethoxyphenyl)-penta-1,4-diene-3-one.

Table 1. ^{1}H and ^{13}C-NMR data of compound **5** ($CDCl_3$)

C no.	δH (∑H; m; *J* Hz) ppm	δC ppm	HMBC (500 MHz)
1	7.7 (1H; d; 16)	143	C6'', C2,C3
2	6.95 (1H; d; 15)	124	C3
3	-	189	-
4	7.1 (1H; d; 16.5)	125	C3, C5,C4'
5	7.4 (1H; d; 12.5)	129	C1'
1'	-	135	-
2'	7.37 (1H; s)	145	C5
3'	-	148	-
3'-OMe	3.8; (3H, s)	56	C4'
4'	-	149	-
4'-OMe	3.9 (3H; s)	56	C3'
5'	6.85 (1H; d; 7)	111	C4', C1'
6'	7.33 (1H; d; 3)	129	C1', C5
1''	-	151	-
2''	7.14 (1H; d; 2)	110	C1'', C6'', C1
3''	7.2 (1H; dd; 7.5)	123	C2'', C1''
4''	7.63 (1H; dd; 7.5)	128	-
5''	6.9 (1H; dd; 10)	120	C4''
6''	7.06 (1H; d; 3.5)	110	C4'', C1'', C1

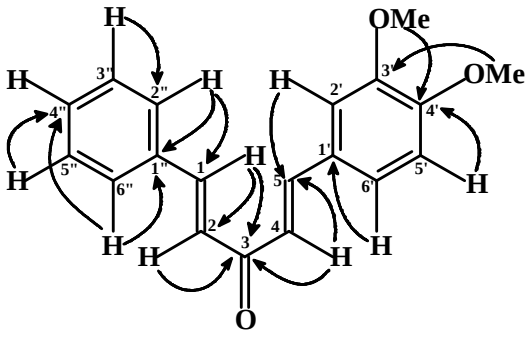

Figure 2. The HMBC of compound **5**

Conclusions

1(E),4(E)-1-phenyl-5-(3',4'-dimethoxyphenyl)-penta-1,4-diene-3-one can be made from acetone, benzaldehyde and 3,4-dimethoxybenzaldehyde by crossed aldol condensation.

Acknowledgement

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References

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